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Some nitrogen-rich heterocycles derivatives as potential explosives and propellants: A theoretical study

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Abstract: Four types of nitrogen-rich heterocycles substituted with $–NO_2$, $–NHNO_2$ and $–C(NO_2)_3$ explosophoric groups were explored as potential explosives and propellants materials. The calculated crystal density (ρ_0) and the condensed phase entalpy change (heat) of formation (Δ_fH) for each of the twelve structures investigated shows that all these derivatives possess high ρ_0 (1.834–1.980 g cm^{-3}) and Δ_fH (605–2130 kJ kg^{-1}) values. Interesting properties such as detonation velocity (D), pressure (p) and specific impulse (I_{SP}) were calculated using the Kamlet–Jacobs method and *ISPBKW* thermochemical code. Detonation velocity and pressure in excess of 8.44 km s^{-1} and 32.87 GPa was obtained in all cases. Furthermore, trinitromethyl substituted derivatives show performance exceeding that of HMX with an estimated D and p in the ranges of 9.32–9.72 km s^{-1} and 40.61–43.82 GPa, respectively. Some $–NO_2$ and $–NHNO_2$ substituted derivatives were shown to be impact-insensitive while retaining good detonation performance and thus are regarded as potential replacement for current RDX-based explosives. Finally, the calculated specific impulse (I_{SP} between 248 and 270 s) of all investigated derivatives indicate that these energetic materials can be considered as possible ingredient in future rocket propellant compositions.

Keywords: energetic materials; detonation performance; specific impulse; Gurney velocity.

INTRODUCTION

The search for new energetic materials (explosives, propellants and pyrotechnics) is an ongoing task all over the world.[1–5] Traditional explosive and propellant formulations relied on carbonaceous backbone (aliphatic and aromatic) based molecules bearing explosophoric groups like nitro ($–NO_2$), nitrate ester ($–ONO_2$) and nitramine ($–NHNO_2$). However, in recent years, much attention has been devoted toward the synthesis of high nitrogen content molecules.[6] For example, high heat of formation (Δ_fH) and crystal density (ρ_0) has been obtained

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by the incorporation of nitrogen rich moiety (*e.g.*, 1,2,4-triazole, tetrazole, 1,2,4,5-tetrazine, etc.).[7] One interesting energetic material is TKX-50 which has been recently synthesized by a research team in Germany.[8] TKX-50 displays excellent detonation performance ($D = 9.70$ km s^{-1}, $p = 42.40$ GPa) which is the direct result of TKX-50 high crystal density ($\rho_0 = 1.88$ g cm^{-3}) and positive heat of formation ($\Delta_f H = 447$ kJ mol^{-1}). Furthermore, TKX-50 possess lower impact sensitivity (20 J) compared to common nitramine based explosives (RDX, HMX and CL-20) which are in the range of 4–7.5 J. Moreover, high-nitrogen molecules are also expected to be promising propellant candidates. In 2010, Zhang *et al.*[9] synthesized a series of 3,4,5-trinitropyrazole-based energetic salts and showed using CHEETAH 5.0[10] thermochemical code that 4-amino-4*H*-1,2,4-triazolium 3,4,5-trinitropyrazolate possess very high specific impulse ($I_{SP} = 270$ s) a value in line with those found in high performance solid rocket propellant formulations. It is a common practice, however, to perform theoretical studies in order to screen out interesting energetic molecules and this before attempting any synthesis. By this strategy, both time and cost can be reduced significantly and only those structures that show good detonation/propellant performance should be considered for synthesis and further characterization.

The goal of this study is to present a series of energetic molecules based on high-nitrogen heterocycles for which the physicochemical, thermodynamic and detonation/propellant properties were predicted. Four types of heterocycles (see Fig. 1) were investigated, namely tetrasubstituted 12*H*-pyrimido[4',5':4,5][1,2,3]-triazolo[2,1-*a*]benzotriazol-5-ium (series A), tetrasubstituted 5*H*,10*H*-bis[1,2,4]-triazolo[1,5-*a*:1',5'-*d*]pyrazine (series B), trisubstituted 5*H*-imidazo[1,2-*b*:3,4-

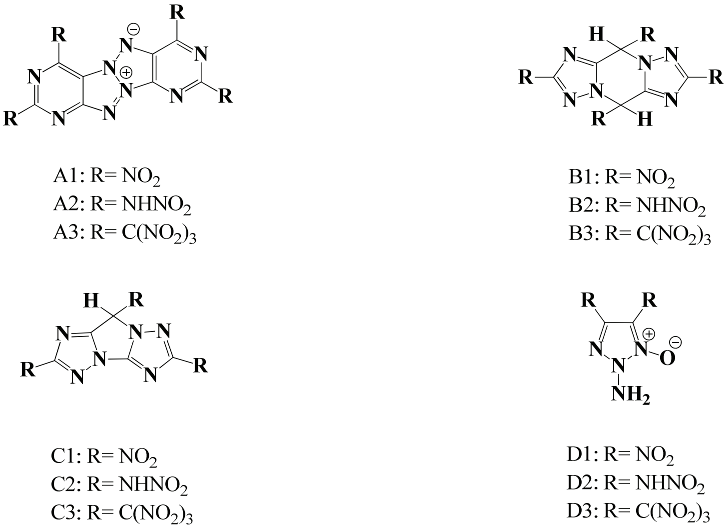

Fig. 1. Structures of the proposed heterocycles as new energetic materials.

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-*b*']bis[1,2,4]triazole (series C) and disubstituted 2-amino-2*H*-1,2,3-triazole, 1-oxide (series D).

METHODS OF CALCULATION

Crystal density (ρ_0) *and heat of formation* (Δ_fH)

Crystal density is of paramount importance in designing energetic materials. It can be shown experimentally[11] that for most powerful high explosive detonation velocity (*D*) is a linear function of ρ_0 while *p* varies with ρ_0^2. In the present study, the simple but reliable group additivity method of Ye and Shreeve[12] was used for the prediction of the crystal density. For 261 explosives containing the elements C-H-N-O-F-S, this approach gives a mean absolute deviation of 0.026 g cm^{-3} and a mean relative absolute error of 1.5 %. As for $\Delta_f H$, Keshavarz[13] devised correlations, Eqs. (1) and (2), based on stoichiometry for the calculation of condensed heat of formation for C-H-N-O containing energetic materials:

$$\Delta_f H = \Delta H_{EC}^0 + 105.0\Delta H_{IEC}^0 - 106.6\Delta H_{DEC}^0 \tag{1}$$

$$\Delta H_{EC}^0 = 32.33a - 39.49b + 92.41c - 63.85d \tag{2}$$

where $\Delta_f H$ is in kJ mol^{-1}, ΔH_{IEC}^0 and ΔH_{DEC}^0 are increasing and decreasing energy corrective terms, respectively, while ΔH_{EC}^0 is the predicted energy content on the basis of elemental composition, and *a*, *b*, *c* and *d* are the number of carbon, hydrogen, nitrogen and oxygen atom, respectively. Equation (1) can be used to predict the heat of formation of a large set of energetic molecules including but not limited to polynitro arenes and polynitro heteroarenes.

*Detonation velocity (*D*) and pressure (*p*)*

When an explosive detonates a propagating detonation wave is established inside the charge which travel at a constant velocity (*D*) determined by a number of factors: crystal density of the explosive, charge diameter, quantity and rate at which the chemical energy is liberated.[14] Another important performance parameter is the detonation pressure (*p*) which represents the brisance or the shattering power of an explosive material.[15] The well-known Kamlet–Jacobs method[16] was used for the prediction of *D* and *p*:

$$D = 1.01\phi^{0.5}(1 + 1.30\rho_0) \tag{3}$$

$$p = 1.558\rho_0^2\phi \tag{4}$$

$$\phi = N\sqrt{MQ} \tag{5}$$

where *D* is in km s^{-1} and *p* in GPa, while *N* and *M* are the number and molecular weight of gaseous detonation products, respectively, and *Q* is the heat of detonation in J g^{-1}.

Impact sensitivities

In order to be useful in real world applications, an energetic material should possess certain degree of insensitivity toward external stimuli such as electric spark, friction and shock impact. An inexpensive test called the drop weight impact test is performed routinely to measure explosives sensitivity. A 2.5 kg weight is released vertically from a predetermined height onto a sample sandwiched between a striker and an anvil. The value generally reported is a mean height for 50 % probability of causing an initiation (h_{50}) or "go". The values of (h_{50}) for all proposed structures shown in Fig. 1 are estimated here following Eqs. (6) and (7):[17]

$$\log h_{50} = \frac{\delta + 44.4167n_{-CNC-} + 102.2749n_{-CNNC-}}{MW} \tag{6}$$

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$$\delta = 46.2923a + 35.6305b - 7.7005c + 7.9425d \qquad (7)$$

where h_{50} is in cm; *a*, *b*, *c* and *d* are the number of C-H-N-O in a given composition, $n_{-\mathrm{CNC}-}$ and $n_{-\mathrm{CNNC}-}$ are the number of $-\mathrm{CNC}-$ and $-\mathrm{CNNC}-$ moieties, *MW* is the molecular weight in g mol^{-1}.

Specific impulse (I_{SP})

Under right conditions, high explosives can be made to burn (or deflagrate) rather than detonate. The gases generated, produce thrust, the force that propel gun projectiles and missiles. The specific impulse (I_{SP}) is used to characterize the energy efficiency of propellant combustion.[18] It has the unit of seconds. The *ISPBKW* code[19] is used for the calculation of I_{SP}. For a given propellant, the equilibrium composition product is obtained at 6.895 MPa chamber pressure (p_{c}) then the combustion gases are permitted to expand isentropically through the rocket motor nozzle to 0.101 MPa ambient pressure (p_{a}). As inputs, *ISPBKW* needs the chemical composition of the propellant and the heat of formation obtained at 0 K.

RESULTS AND DISCUSSION

The results of calculations for the twelve structures of interest (series A, B, C and D) are shown in Table I.

TABLE I. Calculated physiochemical and detonation performance for series A, B, C and D

Cmpd.	ρ_0 g cm^{-3}	$\Delta_{\mathrm{f}}H$ kJ mol^{-1}	$\Delta_{\mathrm{f}}H'$ kJ kg^{-1}	*OB* %	*D* km s^{-1}	*p* GPa	I_{SP} [a] s	h_{50} cm
A1	1.950	716	1826	–32.6	8.44	33.12	256	21
A2	1.906	941	2081	–35.4	8.50	33.17	248	25
A3	1.980	788	975	0	9.32	40.68	260	9
B1	1.881	560	1637	–23.4	8.67	34.24	265	69
B2	1.845	613	1524	–27.8	8.55	32.88	255	69
B3	1.949	459	605	6.3	9.39	40.93	255	14
C1	1.888	603	2130	–25.4	8.65	34.13	265	80
C2	1.854	634	1932	–29.3	8.53	32.87	255	79
C3	1.949	540	907	4.0	9.35	40.61	258	17
D1	1.863	220	1157	0	9.17	38.08	267	7
D2	1.834	262	1190	–7.3	9.00	36.37	270	9
D3	1.942	295	741	16.1	9.72	43.82	250	5
RDX[b]	1.800	62	279	–21.6	8.75	34.70	266[c]	24[d]
HMX[b]	1.900	74	250	–21.6	9.10	39.30	266[c]	26[d]
PETN[b]	1.770	–508	–1607	–10.1	8.30	33.50	265	12[d]

[a]All values were calculated using the *ISPBKW* code[19], otherwise stated; [b]experimental detonation velocity (*D*) and pressure (*p*) of RDX, HMX and PETN were obtained from Mader;[19] [c]the values were obtained from Kuo and Acharya;[20] [d]impact sensitivities are obtained from Storm[21]

*Tetrasubstituted 12*H*-pyrimido[4',5':4,5][1,2,3]triazolo[2,1-*a*]benzotriazol-5-ium (series A)*

The tetraazapentalene ring system represents an interesting building block for insensitive, thermally stable explosive. One such example is the well-known

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TACOT molecule which possesses decomposition temperature of 410°C one of the highest value recorded for an explosive material.[22]

Series A depicted in Fig. 1 exploit the tetraazapentalene system in conjunction with two substituted pyrimidine rings which result in structure having both high nitrogen content (N, 35–50 %) and ρ_0 values (1.906–1.980 g cm^{-3}). The highest and lowest density was obtained with structure bearing trinitromethyl –$C(NO_2)_3$ and nitramino –$NHNO_2$ groups, respectively. It is clear that structure A3 possess the lowest $\Delta_f H$ (975 kJ kg^{-1}) in its series, however, A3 with a zero oxygen balance (OB) and a $\rho_0 = 1.980$ g cm^{-3} has the highest calculated detonation performance (D = 9.32 km s^{-1}, p = 40.68 GPa) and also the highest specific impulse ($I_{SP} = 260$ s). The impact sensitivity of A3 ($h_{50} = 9$ cm) is higher than that of RDX ($h_{50} = 24$ cm) and HMX ($h_{50} = 26$ cm) but is still close to that of PETN[21] ($h_{50} = 12$ cm) keeping in mind that detonation performance of A3 greatly outperform that of PETN[19] ($\rho_0 = 1.77$ g cm^{-3}, D = 8.30 km s^{-1}, p = 33.50 GPa).

On the other hand, A1 and A2 possess detonation performance and impact sensitivity similar to RDX; however, A1 and A2 are denser ($\rho_0 = 1.95$ and 1.906 g cm^{-3} for A1 and A2, respectively, *vs* 1.80 g cm^{-3} for RDX) and, as a consequence, A1 and A2 can be advantageous in size limiting warheads.

It is worth noting that ρ_0 and $\Delta_f H$ for structure A1 have been investigated in an old study using quantum chemical method[23] which gives a $\rho_0 = 1.940$ g cm^{-3} and a $\Delta_f H = 719$ kJ mol^{-1} in close agreement with the result shown in Table I. Furthermore a comparison between the obtained ρ_0 and detonation performance for A1 (1.950 g cm^{-3}, 8.44 km s^{-1} and 33.12 GPa) to that of TACOT[24] (1.820 g cm^{-3}, 7.06 km s^{-1} and 20.30 GPa) obviously shows that the presence of a pyrimidine is advantageous over a phenyl ring for obtaining powerful tetraazapentalene based energetic materials.

*Tetrasubstituted 5*H*,10*H*-bis[1,2,4]-triazolo-[1,5-*a*:1',5'-*d*]pyrazine (series B) and trisubstituted 5*H*-imidazo[1,2-*b*:3,4-*b*']bis[1,2,4]triazole derivatives (series C)*

Unlike the tetraazapentalene nucleus none of the heterocycles of series B and C had been used or investigated as precursors for energetic material preparation. To the best knowledge of the author, 5*H*-imidazo[1,2-*b*:3,4-*b*']bis[1,2,4]triazole heterocycle is unknown while non-energetic 5*H*,10*H*-bis[1,2,4]triazolo[1,5-*a*:1',5'-*d*]pyrazine derivatives can be synthesized by dimerization of 3-phenyl-1*H*-1,2,4-triazole-5-carboxaldehydes (**1**) giving the semiaminals (**2**) or the aminals (**3**) by the reaction of (**2**) with secondary amines as shown in Scheme 1.[25]

Back to the results in Table I, one can notice the increased heat of formation when going from series B to series C and this amounts to 300–500 kJ kg^{-1}. This is not the case when it comes to density as little can be gained in ρ_0 (less than 0.1 g cm^{-3}) with series C being slightly denser than series B. The same trend is

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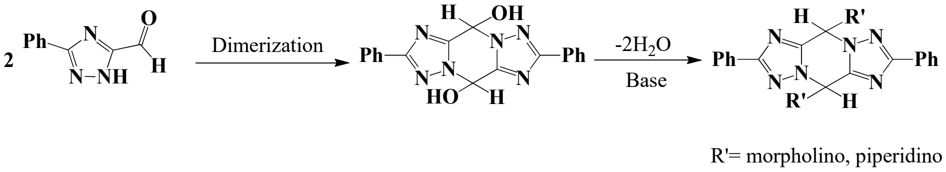
seen when analyzing detonation performance and specific impulse. Like A1 and A2 the detonation performance of $–NO_2$ and $–NHNO_2$ substituted members of series B and C is almost equal to that of RDX (D, 8.53–8.67 km s^{-1} and p, 32.87–34.24 GPa); however, B1, B2, C1 and C2 are far less impact sensitive than RDX and HMX. Both C1 and C2 have a calculated h_{50} of 80 and 79 cm, respectively, and thus nitro and nitramine substituted B and C series can be considered as potential replacement for current RDX based formulations. The trinitromethyl derivatives B3 and C3 are denser and more efficient ($D > 9.30$ km s^{-1} and $p > 40$ GPa) than HMX ($D = 9.10$ km s^{-1} and $p = 39.30$ GPa). Despite, their high performance, B3 and C3 impact sensitivity is still acceptable (h_{50}, 14–17 cm) for future applications.



(1) (2) (3)

Scheme 1. Synthesis of non-energetic derivatives based on series B heterocycle.[25]

Disubstituted 2-amino-2H-1,2,3-triazole, 1-oxide derivatives (series D)

Energetic materials based on the 1,2,3-triazole, 1-oxide moiety have been rarely investigated in the literature. One such example is 2-methyl-4,5-dinitro-2*H*-1,2,3-triazole, 1-oxide (MDNTO) an explosive compound with a moderate crystal density $\rho_0 = 1.730$ g cm^{-3} and a decomposition temperature of 256 °C.[26] In order to gain density, the $–CH_3$ group at position 2 in MDNTO was replaced by $–NH_2$ which results in 7.7 % increase in ρ_0 (structure D1, $\rho_0 = 1.863$ g cm^{-3}). A further increase in density can be accomplished by replacing the two $–NO_2$ in D1 by a $–C(NO_2)_3$ group (structure D3, $\rho_0 = 1.942$ g cm^{-3}). All structures investigated in this series have detonation velocity in excess of 9.00 km s^{-1} with D3 being the most energetic ($D = 9.72$ km s^{-1} and $p = 43.82$ GPa). Furthermore, a remarkable specific impulse value is seen for D2 ($I_{SP} = 270$ s) outperforming RDX and HMX by 4 s. The impact sensitivity of series D is high ranging from 5–9 cm so members of this series can be exploited as lead-free environmentally benign primary explosives or mixed with a polymeric matrix in order to decrease their sensitivity.

HTPB-based plastic-bonded explosives (PBXs)

Explosive materials are seldom used in their pure state. Therefore, in most practical applications, a given explosive is made in formulations where the energetic component is dispersed in an inert/energetic binder (polymeric matrix), so

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as to form what is called a plastic-bonded explosive (PBX). PBXs possess low levels of vulnerability and are characterized by high mechanical strength.[27] Here, the most impact sensitive members of series A, B, C and D are investigated as ingredient in HTPB based PBXs. Their detonation performance as well as their Gurney velocities (metal acceleration ability, $\sqrt{2E_G}$) was calculated and the results are shown in Table II.

For comparison, PBXs made of HMX, RDX, and PETN were included. All PBXs investigated are made with 95/5 explosive/HTPB mass ratio.

TABLE II. Detonation performance as well as acceleration ability of HTBP-based PBXs

Composition	ρ_0 g cm^{-3}	$\Delta_f H$ kJ (100 g)$^{-1}$	D km s^{-1}	P GPa	$\sqrt{2E_G}$ [a] km s^{-1}
A3/HTPB[b], $C_{1.766}H_{0.541}N_{2.356}O_{2.828}$	1.88	91	8.77	35.04	2.88
B3/HTPB, $C_{1.608}H_{0.791}N_{2.261}O_{3.014}$	1.85	74	8.90	35.68	2.93
C3/HTPB, $C_{1.632}H_{0.700}N_{2.400}O_{2.880}$	1.85	85	8.80	34.93	2.90
D3/HTPB, $C_{1.310}H_{1.018}N_{2.392}O_{3.109}$	1.85	69	9.17	37.88	3.02
HMX/HTPB, $C_{1.639}H_{3.107}N_{2.572}O_{2.573}$	1.82	22	8.63	33.24	2.86
RDX/HTPB, $C_{1.639}H_{3.107}N_{2.572}O_{2.573}$	1.73	25	8.34	30.09	2.81
PETN/HTPB, $C_{1.858}H_{2.944}N_{1.207}O_{3.612}$	1.71	–163	8.28	29.46	2.80

[a] Gurney velocity is calculated by following formula:[28] $\sqrt{2E_G} = 0.887\phi^{0.5}\rho_0^{0.4}$; [b] for HTPB,[29] atomic composition is: $C_{7.1102}H_{10.813}N_{0.1071}O_{0.1375}$, $\rho_0 = 0.960$ g cm^{-3}, $\Delta_f H = -31.55$ kJ mol^{-1} at 298.15 K

As Table II shows, formulations based on trinitromethyl substituted derivatives are all superior to current nitramine and nitrate ester compositions. Moreover, interesting high Gurney velocities ($\sqrt{2E_G} \geq 2.88$ km s^{-1}) are obtained with the theoretically proposed composition which makes them candidates for high performance fragmentation warheads.

It is hoped that the addition of HTPB will decrease the impact sensitivity of A3 and D3 to a level of safe handling in future applications.

CONCLUSION

The results shown in Tables I and II prove that the proposed energetic heterocycles are interesting energetic derivatives and several conclusions can be drawn:

1. Four structures, namely B1, B2, C1 and C2 are equally performant to RDX, but on the other hand, their h_{50} values are far more greater (69–80 cm) than that of RDX (h_{50} = 24 cm); thus, $-NO_2$ and $-NHNO_2$ substituted B and C series can be considered as potential replacement for current RDX-based explosives.

2. All investigated heterocycles substituted with $-C(NO_2)_3$ group possess the highest calculated crystal density and the lowest heat of formation on a weight basis. Moreover, the $-C(NO_2)_3$ shows to be the best substitute offering the highest detonation performance ($D \geq 9.10$ km s^{-1}, $p \geq 40.60$ GPa) but also the highest impact sensitivity in their series. Structure B3 and C3 are more efficient than

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HMX while retaining acceptable impact sensitivity (h_{50}, 14–17 cm). Furthermore, trinitromethyl substituted structures of all the series studied were investigated in PBX formulations. The PBXs are of 95/5 explosive/HTPB mass ratio and the calculation shows that the detonation performance of all these formulations are superior to similar PBXs based on HMX, RDX and PETN. Finally, these HTPB-based formulations can find their way in future high performance warheads due to their high Gurney velocities ($\sqrt{2E_G}$, 2.88–3.02 km s^{-1}).

3. All derivatives investigated in this study show high calculated I_{SP} values, ranging from 248 to 270 s.

NOMENCLATURE

CL-20	2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0$^{5.9}$.0$^{3.11}$]dodecane
HMX	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine
HTPB	Hydroxy-terminated polybutadiene
PETN	Pentaerythritol tetranitrate
RDX	Hexahydro-1,3,5-trinitro-1,3,5-triazine
TACOT	1,3,7,9-tetranitro-6*H*-benzotriazolo[2,1-*a*]-benzotriazole-5-ium, inner salt
TKX-50	Dihydroxylammonium 5,5'-bi-1*H*-tetrazole-1,1'-diolate

ИЗВОД

НЕКИ АЗОТОМ БОГАТИ ХЕТЕРОЦИКЛИЧНИ ДЕРИВАТИ КАО ПОТЕНЦИЈАЛНИ ЕКСПЛОЗИВИ И ГОРИВА: ТЕОРИЈСКА АНАЛИЗА

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Испитивана су четири типа азотом богатих хетероцикличних деривата супституисаних са $-NO_2$, $-NHNO_2$ и $-C(NO_2)_3$ експлозофорним групама као потенцијани експлозиви и горивни материјали. Израчунавања су показала да свих 12 испитиваних структура имају високе вредности густине кристала (1,834–1,980 g cm^{-3}) и промену енталпије (топлоту) формирања кондензоване фазе (605–2130 kJ kg^{-1}). Важна својства, као што су брзина детонације (D), притисак (p) и специфични импулс су израчуната коришћењем Kamlet–Jacobs методе и *ISPBKW* термохемијског кода. Вредности брзине детонације су биле веће од 8,44 km s^{-1}, а притиска од 32,87 GPa. Перформансе тринитрометил супституисаних деривата превазилазе перформансе HMX, са вредностима D од 9,32 до 9,72 km s^{-1} и p од 40,61 до 43,82 GPa. Неки $-NO_2$ и $-NHNO_2$ супституисани деривати су се показали као неосетљиви на удар, али су задржали добре детонаторске перформансе, па потенцијално могу заменити постојеће експлозиве на бази RDH. Израчунате вредности специфичног импулса (између 248 и 270 s) за све испитиване деривате указују да ови енергетски материјали могу бити састојци будућих ракетних горива.

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